

ON THE COMPUTATIONAL STABILITY OF NUMERICAL SOLUTIONS OF TIME-DEPENDENT NON-LINEAR GEOPHYSICAL FLUID DYNAMICS PROBLEMS

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ABSTRACT

The satisfactory numerical solution of the equations of fluid dynamics applicable to atmospheric and oceanic problems characteristically requires a high degree of computational stability and accurate conservation of certain statistical moments. Methods for satisfying these requirements are described for various systems of equations typical of low Mach number fluid dynamics systems, and are investigated in detail as applied to the two-dimensional, inertial-plane equation for conservation of vorticity in a frictionless non-divergent fluid.

The conservation and stability properties of the spatial differencing methods devised by A. Arakawa are investigated by means of spectral analysis of the stream function into finite Fourier modes. Any of two classes of linear and quadratic conserving schemes are shown to eliminate the non-linear instability discussed by Phillips, although the "aliasing" error remains. Stability related to the time derivative term is investigated through analytic and numerical solutions of a limited-component system of finite spectral equations, equivalent to one of the quadratic conserving difference schemes, and a number of first and second order representations of the time derivative term are tested separately. The commonly used midpoint rule ("leapfrog") method is shown to be unstable in some cases. Of the stable methods, that devised by Miyakoda and the second order Adams-Bashforth method exhibit satisfactory accuracy, while those due to Matsuno, and Lax and Wendroff are much less accurate.

A systematic derivation of the Arakawa difference schemes is contained in an appendix, which shows their unique satisfaction of certain prescribed accuracy and conservation properties.

1. INTRODUCTION

In the last 10 years numerical methods have been used with increasing frequency and success for solving non-linear initial-value boundary-value problems in fluid dynamics. The availability of high-speed electronic computers has probably been the major factor in the success attained, since many of the problems had been properly posed for many years. Much of the numerical analysis necessary to satisfactorily formulate these problems for computational solutions also dates back to pre-electronic eras. In recent years, however, it has become clear that methods of numerical formulation must, to some extent, be tailored to the nature of the expected solution. Thus in spite of the almost universal application of the Navier-Stokes equations, numerical solutions involving shock waves should evidently be obtained in a rather different manner from those pertaining to, for example, unsteady thermal convection. The finite difference methods developed at the Courant Institute (Courant, Isaacson, and Rees [5]; Lax and Wendroff [13]; Richtmyer [21]) may be quite appropriate for high Mach number problems involving a single energetic "event". They often are severely inadequate, however, when applied to an atmospheric general circulation problem, in which accurate calculation

of the statistical parameters of a number of sequential, and somewhat random, events is the primary requirement. In general, atmospheric and oceanographic equations are highly non-linear, and useful computation often requires that momentum, energy, circulation, heat, and other variables be created, transformed, and dissipated through several energetic cycles with a minimum of consistent, i.e. non-random, computational error. Meteorologists can ordinarily tolerate random error magnitudes up to the error limit of the rather poorly known initial conditions. Few competent meteorologists expect to be able to make detailed daily weather forecasts, by computer or otherwise, six months in advance, but a numerical calculation in which 10 percent of the mass of the atmosphere is lost through computational error during this period may be highly suspect in its other statistical conclusions. We thus may summarize the special requirements of many geophysical fluid calculations to be accurate conservation of linear and quadratic integral properties and great computational stability, perhaps to the exclusion of optimum accuracy in shape and phase representation. Somewhat the same requirements might be expected to prevail in some other low Mach number problems of the more classical type, such as the Karman vortex street calculations recently performed by Fromm and Harlow [9]. By contrast, however, operational weather forecasting models seem to require essentially the opposite properties.

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It is well known that finite representation of fluid motions by means of truncated Fourier spectra allows high accuracy, stability, and conservation of all appropriate quantities, but at great cost in computational effort. The number of multiplications required to compute non-linear interactions increases as the square of the number of components, as compared to a linear increase in finite difference formulations. Spatial differencing formulas recently developed by Arakawa [1], and Fromm [8] appear to offer most of the advantages of the spectral methods within a grid point formulation. These formulas have the property of requiring conservation of linear and quadratic quantities within the advection terms and appear, to a certain extent, to insure computational stability. Although they have already been used successfully in several different problems (Lilly [14], Bryan [2], Mintz and Arakawa [17], Fromm and Harlow [9]), very little is known of the general properties of these methods. This study is an attempt to compare different methods, and assess their stability in a systematic way.

In section 2, linear and quadratic conserving spatial differencing schemes are exhibited for two systems of hydrodynamic equations which typify many systems arising in meteorological and oceanographic problems. In section 3 the schemes appropriate for one of the hydrodynamic systems, consisting simply of a frictionless barotropic vorticity equation, are examined and compared in some detail by means of analysis into finite Fourier spectral equations. It is shown that the quadratic conserving schemes allow construction of one or more Liapunov functions, the existence of which assures stability for the continuous time equations. Section 4 contains examples of limited component sets, similar to those used by Phillips [19] and Lorenz [15], which more simply illustrate the effect of application of the conserving schemes.

In sections 5 and 6 methods of numerical approximation of the time derivative are compared through analytic and numerical solutions of one of the limited component Fourier spectral sets previously derived. The known tendency toward instability of the midpoint rule, or "leapfrog," method is illustrated and partially explained. Other methods considered are mostly stable but show widely varying accuracy.

A systematic derivation of the Arakawa spatial difference scheme and related linear-quadratic conserving schemes for the barotropic vorticity equation is presented in the appendix.

2. SPATIAL DIFFERENCE SCHEMES

Perhaps the simplest flow of general interest in meteorology and oceanography is that of a frictionless incompressible homogeneous fluid, constrained to two-dimensional motion between fixed parallel upper and lower boundaries. The equations of motion reduce to an equation for conservation of the vorticity component perpendicular to the

boundaries, that is

$$\frac{\partial \zeta}{\partial t} = -J(\psi, \zeta) = -\frac{\partial \psi}{\partial x} \frac{\partial \zeta}{\partial y} + \frac{\partial \psi}{\partial y} \frac{\partial \zeta}{\partial x} \quad (2.1)$$

where ψ is the streamfunction, $\zeta = \partial^2 \psi / \partial x^2 + \partial^2 \psi / \partial y^2$, and J symbolizes the two-dimensional Jacobian. From this equation it is easily shown that kinetic energy, $(\nabla \psi)^2 / 2$, and any function of ζ are conserved in the flow; that is, that their integrals over a fixed region in space can only change by transport through the boundaries of the region.

It is unlikely that any finite representation of the Jacobian can conform to all these integral conditions, but Arakawa [1] has developed a class of second-order finite difference schemes which conserve the vorticity and one or both of the quadratic quantities, kinetic energy and squared vorticity. The schemes are conveniently described by use of three fundamental formulas for the Jacobian, J_1 , J_2 , and J_3 , as follows:

$$\begin{aligned} J_1 &= \delta_x \bar{\psi}^x \delta_y \bar{\zeta}^y - \delta_y \bar{\psi}^y \delta_x \bar{\zeta}^x \\ J_2 &= \delta_x (\bar{\psi} \delta_y \bar{\zeta}^y)^x - \delta_y (\bar{\psi} \delta_x \bar{\zeta}^x)^y \\ J_3 &= -\delta_x (\bar{\zeta} \delta_y \bar{\psi}^y)^x + \delta_y (\bar{\zeta} \delta_x \bar{\psi}^x)^y. \end{aligned} \quad (2.2)$$

The notation, used in a previous paper (Lilly [14]), is defined by the following identities:

$$\begin{aligned} \delta_x F(x) &= \frac{1}{\Delta x} \left[F\left(x + \frac{\Delta x}{2}\right) - F\left(x - \frac{\Delta x}{2}\right) \right], \\ \overline{F(x)}^x &= \frac{1}{2} \left[F\left(x + \frac{\Delta x}{2}\right) + F\left(x - \frac{\Delta x}{2}\right) \right] \\ \delta_x \overline{F(x)}^x &= \delta_{2x} F(x) = \frac{1}{2\Delta x} [F(x + \Delta x) - F(x - \Delta x)] \end{aligned} \quad (2.3)$$

where $F(x)$ is any function of the discrete variable x and Δx is the grid interval. These formulas are derived in the appendix and it is shown there that J_1 conserves vorticity, J_2 conserves vorticity and its square, J_3 conserves vorticity and kinetic energy, and the combination $J_A = (J_1 + J_2 + J_3)/3$ conserves all three. It is shown in the appendix that J_A is unique in its properties within a certain class of approximations, but that J_1 , J_2 , and J_3 are not, since any linear combination of J_A with either of the others retains the latter's properties.

The scheme designated J_1 is often called the "usual" difference scheme and was used in early numerical weather forecasting (Charney, Fjörtoft, and Von Neumann [3]). Phillips [19] showed that the scheme is unconditionally unstable to disturbances in certain high frequency modes. J_3 was used by Bryan [2] in ocean current calculations and by Lilly [14] and Deardorff [6] in convective problems. Fromm [8] developed J_3 and $(J_1 + J_3)/2$ independently for use in computational simulation of flow past a cylinder. Mintz and Arakawa [17] used J_A in general circulation calculations. In these applications the use of the quadratic conserving forms reportedly eliminated or greatly

reduced all tendencies toward computational instability. In some cases, however, the difference method used for approximating the *time* derivative apparently led to a slow instability of the inviscid equations.

If the upper boundary constraint in the previously discussed flow is replaced by a vanishing stress condition, the two-dimensional equations may be written in a form which is typical of many other geophysical fluid dynamics systems, including that of recent general circulation calculations by Smagorinsky [23]. If h is the height of the free surface, then the frictionless two-dimensional equations of fluid momentum and continuity are:

$$\frac{\partial}{\partial t}(hu) + \frac{\partial}{\partial x}(hu^2) + \frac{\partial}{\partial y}(huv) + gh \frac{\partial h}{\partial x} = 0 \quad (2.4)$$

$$\frac{\partial}{\partial t}(hv) + \frac{\partial}{\partial x}(huv) + \frac{\partial}{\partial y}(hv^2) + gh \frac{\partial h}{\partial y} = 0 \quad (2.5)$$

$$\frac{\partial h}{\partial t} + \frac{\partial}{\partial x}(hu) + \frac{\partial}{\partial y}(hv) = 0 \quad (2.6)$$

The mass per unit area, ρh , and total energy per unit area, $\rho(hu^2 + hv^2 + gh^2)/2$, are conserved in this set (density, ρ , is a constant), as are the momentum components except for boundary pressure forces.

A system of finite difference equations which preserves the above conservative properties is the following:

$$\frac{\partial}{\partial t}(\bar{h}^x u) + \delta_x(\bar{h}^x \bar{u}^x) + \delta_y(\bar{h}^x \bar{u}^y) + g\bar{h}^x \delta_x h = 0 \quad (2.7)$$

$$\frac{\partial}{\partial t}(\bar{h}^y v) + \delta_y(\bar{h}^y \bar{v}^y) + \delta_x(\bar{h}^y \bar{v}^x) + g\bar{h}^y \delta_y h = 0 \quad (2.8)$$

$$\frac{\partial h}{\partial t} + \delta_x(\bar{h}^x u) + \delta_y(\bar{h}^y v) = 0. \quad (2.9)$$

Verification of the energy conservation property can be readily obtained by methods outlined in a previous paper (Lilly [14]). Upon taking the finite difference curl of (2.7) and (2.8) in the case of h constant, the advective terms become identical to J_3 in (2.2). Since the square of the potential vorticity per unit area, $\rho \zeta^2/h$, is also conserved in (2.4)–(2.6), finite difference forms similarly related to J_2 and J_4 should also exist for this system, but the possibility has not been explored. It may be noted that h , u , and v in (2.7)–(2.9) are defined at different locations in the mesh. This is not necessary for the conservation properties, since a closely related system can be devised in which all variables are located at the same points. The above system minimizes truncation error in the terms which contribute to linear gravitational oscillations.

In most practical or theoretical initial value problems to which numerical methods are applied, the equations, variables, or coordinates exhibit greater complexities than are presented in (2.1) or (2.7)–(2.9). In most cases it appears that the difference equations can be

altered and/or added to in a fairly mechanical manner to preserve the desired integral properties, as with the examples given by Arakawa, Bryan, and Lilly. Most numerical forecasting models, including primitive equations models in which a condition of two- or three-dimensional non-divergence exists, can be treated with schemes closely related to those described for (2.1). The compressible Navier-Stokes equations and the equations of large-scale motion allowing external gravity waves are of the form of (2.4)–(2.6). Conservative equations of a scalar, say T , can be written using either the form of $(J_1 + J_3)/2$, for incompressible flow, or the following equivalent form appropriate to compressible flow:

$$\frac{\partial}{\partial t}(hT) + \delta_x(\bar{h}^x u \bar{T}^x) + \delta_y(\bar{h}^y v \bar{T}^y) = 0. \quad (2.10)$$

These forms conserve T^2 or hT^2 , respectively, within the advection terms.

3. SPECTRAL ANALYSIS

The equations of motion in finite Fourier spectral forms have been used both in diagnostic studies and in simplified geophysical models. In this section we derive and investigate the non-linear terms in spectral form for the finite difference Jacobian expressions J_1 , J_2 , J_3 , and J_4 above. The investigation shows that the truncation errors involved in the finite difference spectra are of three different types, only two of which are removable by increasing the order of the difference equations. The third type of error, commonly known as aliasing, is responsible for a form of instability demonstrated by Phillips [19].

Although Phillips called it a nonlinear instability, Miyakoda [18] (p. 175) showed that it can occur also in linear equations with nonconstant coefficients. The unstable behavior of this error is eliminated in the Arakawa differencing schemes, by compensating triad interactions, as in the analytic spectral equations. We may express the stream function, vorticity, etc., as a series of complex exponential functions with vector wave number $\mathbf{M} = im + jn$, as follows:

$$\psi = \sum_{\mathbf{M}} A_{\mathbf{M}} e^{im(\mathbf{M} \cdot \mathbf{R})} = \sum_{\mathbf{M}} \psi_{\mathbf{M}} \quad (3.1)$$

where $\mathbf{R} = ix + jy$, $im = \sqrt{-1}$ and the summation is over a finite set of wave numbers.

Approximately following Lorenz [15], we write for the vorticity

$$\zeta = - \sum_{\mathbf{M}} |\mathbf{M}|^2 A_{\mathbf{M}} e^{im(\mathbf{M} \cdot \mathbf{R})} = - \sum_{\mathbf{M}} |\mathbf{M}|^2 \psi_{\mathbf{M}} \quad (3.2)$$

and obtain the analytic Jacobian in the vector product form

$$J(\psi, \zeta) = \sum_{\mathbf{M}', \mathbf{M}''} (\mathbf{k} \cdot \mathbf{M}' \times \mathbf{M}'') |\mathbf{M}''|^2 \psi_{\mathbf{M}'} \psi_{\mathbf{M}''} \quad (3.3)$$

or, in a symmetric form

$$J(\psi, \zeta) = \frac{1}{2} \sum_{\mathbf{M}', \mathbf{M}''} (\mathbf{k} \cdot \mathbf{M}' \times \mathbf{M}'') (|\mathbf{M}''|^2 - |\mathbf{M}'|^2) \psi_{\mathbf{M}'} \psi_{\mathbf{M}''}. \quad (3.4)$$

Considering now the finite difference equations, we must introduce certain substitutions for the wave numbers appearing in the derivative expressions. We expand the notation defined in (2.3) to include the finite gradient and Laplacian operators

$$\begin{aligned} \bar{\nabla} F &= i \delta_x \bar{F}^x + j \delta_y \bar{F}^y \\ \nabla^2 F &= \delta_{xx} F + \delta_{yy} F \\ &= \delta_x (\delta_x F) + \delta_y (\delta_y F) \end{aligned} \quad (3.5)$$

and note that after operation on a complex exponent, sines of the wave numbers appear, e.g.,

$$\bar{\nabla} e^{im(\mathbf{M} \cdot \mathbf{R})} = \mathbf{S}(\mathbf{M}) i m e^{im(\mathbf{M} \cdot \mathbf{R})} \quad (3.6)$$

where

$$\mathbf{S}(\mathbf{M}) = \frac{i \sin m\Delta + j \sin n\Delta}{\Delta} \quad (3.7)$$

and

$$\nabla^2 e^{im(\mathbf{M} \cdot \mathbf{R})} = -4 |\mathbf{S}(\mathbf{M}/2)|^2 e^{im(\mathbf{M} \cdot \mathbf{R})}.$$

Although it is not essential to the analysis, we have assumed that the grid is isotropic, so that $\Delta = \Delta x = \Delta y$. The vector $\mathbf{S}(\mathbf{M})$ approaches \mathbf{M} for small wave numbers, but it obviously does not possess distributive properties, i.e.,

$$\mathbf{S}(\mathbf{M}_1 + \mathbf{M}_2) \neq \mathbf{S}(\mathbf{M}_1) + \mathbf{S}(\mathbf{M}_2).$$

We now may write the finite difference Jacobian expressions J_1 , J_2 , and J_3 in spectral form as follows:

$$\begin{aligned} J_1 &= \mathbf{k} \cdot \bar{\nabla} \psi \times \bar{\nabla} \zeta = 2 \sum_{\mathbf{M}', \mathbf{M}''} \mathbf{k} \cdot [\mathbf{S}(\mathbf{M}') \times \mathbf{S}(\mathbf{M}'')] \\ &\quad \left\{ \left| \mathbf{S}\left(\frac{\mathbf{M}''}{2}\right) \right|^2 - \left| \mathbf{S}\left(\frac{\mathbf{M}'}{2}\right) \right|^2 \right\} \psi_{\mathbf{M}'} \psi_{\mathbf{M}''} \end{aligned} \quad (3.8)$$

$$\begin{aligned} J_2 &= \mathbf{k} \cdot \bar{\nabla} \times (\psi \bar{\nabla} \zeta) = 2 \sum_{\mathbf{M}', \mathbf{M}''} \mathbf{k} \cdot \mathbf{S}(\mathbf{M}' + \mathbf{M}'') \\ &\quad \times \left\{ \mathbf{S}(\mathbf{M}'') \left| \mathbf{S}\left(\frac{\mathbf{M}''}{2}\right) \right|^2 + \mathbf{S}(\mathbf{M}') \left| \mathbf{S}\left(\frac{\mathbf{M}'}{2}\right) \right|^2 \right\} \psi_{\mathbf{M}'} \psi_{\mathbf{M}''} \end{aligned} \quad (3.9)$$

$$\begin{aligned} J_3 &= -\mathbf{k} \cdot \bar{\nabla} \times (\zeta \bar{\nabla} \psi) = -2 \sum_{\mathbf{M}', \mathbf{M}''} \mathbf{k} \cdot \mathbf{S}(\mathbf{M}' + \mathbf{M}'') \\ &\quad \times \left\{ \mathbf{S}(\mathbf{M}'') \left| \mathbf{S}\left(\frac{\mathbf{M}'}{2}\right) \right|^2 + \mathbf{S}(\mathbf{M}') \left| \mathbf{S}\left(\frac{\mathbf{M}''}{2}\right) \right|^2 \right\} \psi_{\mathbf{M}'} \psi_{\mathbf{M}''}. \end{aligned} \quad (3.10)$$

Finally, after summing the above three expressions we may write the averaged form, J_A , as

$$\begin{aligned} J_A &= (J_1 + J_2 + J_3)/3 = \frac{2}{3} \sum_{\mathbf{M}', \mathbf{M}''} \mathbf{k} \cdot \{ \mathbf{S}(\mathbf{M}') \times \mathbf{S}(\mathbf{M}'') \\ &\quad + [\mathbf{S}(\mathbf{M}' + \mathbf{M}'')] \times [\mathbf{S}(\mathbf{M}'') - \mathbf{S}(\mathbf{M}')] \} \cdot \left\{ \left| \mathbf{S}\left(\frac{\mathbf{M}''}{2}\right) \right|^2 \right. \\ &\quad \left. - \left| \mathbf{S}\left(\frac{\mathbf{M}'}{2}\right) \right|^2 \right\} \psi_{\mathbf{M}'} \psi_{\mathbf{M}''}. \end{aligned} \quad (3.11)$$

The conservation properties are demonstrable upon consideration of the triad interactions obtained in forming the energy and squared vorticity equations. Thus in the product $\psi_{-\mathbf{M}'-\mathbf{M}''} J_A$ the complex exponential reduces to unity and the product has a nonvanishing spatial integral proportional to the amplitude product $A_{-\mathbf{M}'-\mathbf{M}''} A_{\mathbf{M}'} A_{\mathbf{M}''}$ multiplied by the interaction coefficient of (3.11). Upon cyclically transposing \mathbf{M}' , \mathbf{M}'' , and $-\mathbf{M}'-\mathbf{M}''$ the three interaction coefficients obtained sum to zero, proving kinetic energy conservation within the triad. A similar result is obtained for the products which lead to conservation of squared vorticity. J_2 and J_3 may respectively be shown to conserve squared vorticity and kinetic energy alone. The spectral equations do not in themselves determine whether the non-conserved properties grow or diminish, as that depends on phase and amplitude conditions for a given case.

In comparing the finite expressions (3.8)–(3.11) with the analytic Jacobian (3.3) or (3.4) one may segregate the differences, or truncation errors, into three different classes, here designated as first derivative errors, second derivative errors, and aliasing errors. First derivative errors are introduced by the approximation of \mathbf{M} by $\mathbf{S}(\mathbf{M})$, that is the replacement of wave numbers by their sines. These errors are quantitatively present in all interactions, and introduce a qualitative effect when two wave numbers, \mathbf{M}' and \mathbf{M}'' are parallel. Equation (3.3) shows that, for the analytic equations, the interaction coefficient disappears and no new component is generated, but this is not true for (3.8)–(3.11). These errors may be reduced by using a higher order difference scheme, for which $\mathbf{S}(\mathbf{M})$ is replaced by the Fourier sine series converging toward \mathbf{M} in the range from $-\pi/\Delta$ to π/Δ in each coordinate direction. Outside this range the series becomes periodic, but the resulting error should be classified as aliasing.

Second derivative errors occur in the approximation to the factor $\mathbf{M} \cdot \mathbf{M}$ by $4|\mathbf{S}(\mathbf{M}/2)|^2$, associated with the computation of vorticity from the stream function. As with the first derivative errors they occur to some extent in all interactions and also cause qualitative errors in certain cases. Equation (3.4) shows that no interaction should exist for wave numbers of equal magnitude, that is with $|\mathbf{M}'| = |\mathbf{M}''|$. Again this property is not accurately represented in the finite approximations, as can be shown, for example, by choosing two components with wave numbers $m'\Delta = 3\pi/5$, $n'\Delta = 4\pi/5$ and $m''\Delta = \pi$, and $n''\Delta = 0$. By use of a 5-point Laplacian we obtain a value of $|\mathbf{S}(\mathbf{M}'/2)|^2 - |\mathbf{S}(\mathbf{M}''/2)|^2 \approx 0.559/\Delta^2$. Again these errors can be reduced by expanding the network of points to compute the Laplacian.

The aliasing error is not explicitly apparent in the spectral equations, but arises instead from the wave number limits representable in a finite mesh of grid points. The highest wave number unambiguously representable in the x -direction is $m = \pi/\Delta$, while higher values than this are misinterpreted as $-\pi/\Delta + m$. Thus the interactions

symbolically represented in equations (2.8)–(2.11) include not only those corresponding essentially to those of the analytic formulation but also a complete set of spurious interactions involving reflections of one or both components. Since these interactions can involve low as well as high wave number components they could conceivably cause serious distortion of the solution for cases in which energy is dispersed throughout the resolvable modes. Later, however, we see that their magnitude is typically about equal to that of the derivative errors. Since the spurious interactions occur in triads they do not alter the quadratic conservation properties of J_1 , J_2 , and J_3 .

The conservation of spatially integrated kinetic energy and squared vorticity in (2.1) is equivalent to constancy of the corresponding sums of quadratic amplitude components, i.e.

$$\iint \psi \nabla^2 \psi dx dy \propto \sum_{\mathbf{M}} |\mathbf{M}|^2 A_{\mathbf{M}} A_{-\mathbf{M}} = \text{constant}$$

$$\iint (\nabla^2 \psi)^2 dx dy \propto \sum_{\mathbf{M}} |\mathbf{M}|^4 A_{\mathbf{M}} A_{-\mathbf{M}} = \text{constant}. \quad (3.12)$$

The corresponding properties of the finite Jacobian lead to one or both of the similar finite difference requirements:

$$\sum_{x,y} \psi \nabla^2 \psi \propto 4 \sum_{\mathbf{M}} \left| S\left(\frac{\mathbf{M}}{2}\right) \right|^2 A_{\mathbf{M}} A_{-\mathbf{M}} = \text{constant}$$

$$\sum_{x,y} (\nabla^2 \psi)^2 \propto 16 \sum_{\mathbf{M}} \left| S\left(\frac{\mathbf{M}}{2}\right) \right|^4 A_{\mathbf{M}} A_{-\mathbf{M}} = \text{constant}. \quad (3.13)$$

The existence of these constant quadratic sums clearly puts bounds on the magnitude of the stream function and all of its finite derivatives either in grid or finite-dimensional phase space. Somewhat more specific statements can be made upon recognition that either of the conditions of either (3.12) or (3.13) is sufficient to define a Liapunov function, whose existence ensures Liapunov stability about the phase-space origin of the corresponding differential equations. A positive definite function $V(x_i)$ of phase space components x_i about an arbitrary origin is defined (see, e.g. LaSalle and Lefschetz [12]) to be a Liapunov function if:

- $V(x_i)$ is continuous together with its first partial derivatives in a certain open region Ω about the origin.
- $V(0) = 0$.
- Outside the origin (and always in Ω) $V(x_i)$ is positive.
- $dV/dt \leq 0$ in Ω .

The energy and squared vorticity functions of the amplitude components $A_{\mathbf{M}}$ are positive definite since $A_{-\mathbf{M}}$ is the complex conjugate of $A_{\mathbf{M}}$ (because ψ is real) and all the other conditions are obviously satisfied including the equality of (d).

4. LIMITED COMPONENT SYSTEMS

In several previous investigations of the behavior and stability properties of meteorological equations it has

been useful to consider systems of equations of a few interacting phase components. Although all the important qualitative and quantitative properties of the Arakawa difference schemes seem to be obtainable from the general Fourier expansions, it is nevertheless interesting to construct limited component systems for comparison with previously investigated examples.

Phillips [19] discovered a two-component (three coefficient) system whose interactions in J_1 are entirely self contained, that is, no new components are created. All the interactions involve aliasing and are therefore spurious, and the system would be steady state in an analytic but truncated phase space formulation. Phillips showed that these spurious interactions lead to unconditional computational instability. The components are the following:

$$\psi = \left(C \cos \frac{\pi i}{2} + S \sin \frac{\pi i}{2} + U \cos \pi i \right) \sin \frac{2\pi j}{3} \quad (4.1)$$

Applying J_1 to this system one obtains the following coefficient equations:

$$\frac{dC}{dt} = \sigma_1 U S$$

$$\frac{dS}{dt} = \sigma_1 U C$$

$$\frac{dU}{dt} = 0 \quad (4.2)$$

where

$$\sigma_1 = \frac{\sin \frac{\pi}{2} \sin \frac{2\pi}{3}}{2\Delta^2} \cdot \frac{\sin^2 \frac{\pi}{2} - \sin^2 \frac{\pi}{4}}{\sin^2 \frac{\pi}{4} + \sin^2 \frac{\pi}{3}} = \frac{\sqrt{3}}{10\Delta^2}.$$

The solutions of (4.2) have exponentially growing parts for any non-zero U and are therefore unstable. If first and second derivative errors were eliminated (4.2) would be unchanged in form but with σ_1 increased by a factor of about 5.

Upon substitution of (4.1) into J_2 the corresponding coefficient equations became:

$$\frac{dC}{dt} = \sigma_2 U S$$

$$\frac{dS}{dt} = \sigma_2 U C$$

$$\frac{dU}{dt} = -k_2 \sigma_2 C S \quad (4.3)$$

where

$$\sigma_2 = -7\sqrt{3}/20\Delta^2$$

and

$$k_2 = (5/7)^2.$$

The solutions of (4.3) are periodic in most cases, and may be expressed in terms of Jacobian elliptic functions. Asymptotic solutions exist for $|C|=|S|$, while for $|C|, |S| \ll |U|$ the elliptic functions approach sinusoidal behavior. A similar behavior occurs in the energy conserving system J_3 , with coefficients $\sigma_3 = \sqrt{3}/4\Delta^2$, $k_3 = 5/7$. When the components are substituted in J_A , however, all interactions vanish and we obtain the trivial equations $dC/dt = dS/dt = dU/dt = 0$. In these cases also the first and second derivative errors introduce only quantitative effects (no effect in J_A).

It is evident that, although aliasing errors remain, the type of instability demonstrated by Phillips is removed by any of the quadratic conserving schemes. The removal in J_2 and J_3 is effected by introduction of a third spurious interaction which combines with the other two to form a triad. In J_A the form of the interaction matrix seems to forbid existence of any self-contained two-component sets with non-vanishing interactions. None, at any rate, has been found. Four-component sets exist in abundance. Although their behavior is slightly more complicated, it is of interest to examine one such set closely related to Lorenz' "maximum simplification" equations. The motive for this is to see how the three types of truncation errors, and especially the aliasing error, affect a set in which real and spurious (aliasing) interactions are both present.

Lorenz [15] performed time integrations on a three-component set of Fourier components which he called the "maximum simplification" set. If we add one additional component to this set, and specify the wave numbers, it can be directly compared to a corresponding self-contained finite difference set. The components used are:

$$\begin{aligned}\psi_A &= A \cos \frac{\pi i}{2}, \psi_B = B \cos \frac{2\pi j}{3}, \\ \psi_C &= C \sin \frac{\pi i}{2} \sin \frac{2\pi j}{3}, \psi_D = D \cos \pi i \cos \frac{2\pi j}{3}.\end{aligned}\quad (4.4)$$

The analytic Jacobian leads to component equations as follows:

$$\begin{aligned}\frac{dA}{dt} &= \frac{\pi^2}{3\Delta^2} \left[-\frac{1}{2} BC - \left(\frac{3}{4}\right) CD \right] \\ \frac{dB}{dt} &= \frac{\pi^2}{3\Delta^2} \left[\frac{1}{2} AC \right] \\ \frac{dC}{dt} &= \frac{\pi^2}{3\Delta^2} \left[-\frac{17}{25} AB + \frac{43}{25} \left(\frac{1}{2}\right) AD \right] \\ \frac{dD}{dt} &= \frac{\pi^2}{3\Delta^2} \left[-\frac{4}{13} \left(\frac{1}{2}\right) AC \right]\end{aligned}\quad (4.5)$$

while J_A leads to the similar relations

$$\frac{dA}{dt} = \frac{\sqrt{3}}{2\Delta^2} \left[-\frac{1}{2} BC - \frac{1}{3} \left(\frac{1}{2}\right) CD \right]$$

$$\begin{aligned}\frac{dB}{dt} &= \frac{\sqrt{3}}{2\Delta^2} \left[\frac{1}{2} AC \right] \\ \frac{dC}{dt} &= \frac{\sqrt{3}}{2\Delta^2} \left[-\frac{1}{5} AB + \left(\frac{1}{3}\right) AD \right] \\ \frac{dD}{dt} &= \frac{\sqrt{3}}{2\Delta^2} \left[-\frac{3}{7} \left(\frac{1}{6}\right) AC \right].\end{aligned}\quad (4.6)$$

The common factors to the left of the brackets in (4.5) and (4.6) are affected by first derivative errors in the latter, while the digital fractions inside parentheses are affected by aliasing errors. All other terms are affected by second derivative errors except for the first inside the bracket in the dA/dt and dB/dt equations. By comparison of the corresponding error magnitudes we see that first derivative errors are, in general, largest, and the second derivative and aliasing errors somewhat smaller. Thus it appears that some improvement of accuracy could be secured by using a third-order expression for the first spatial derivatives as is now done in routine numerical forecasting (Shuman and Vanderman [22]). Further refinements would be ineffective because of the remaining aliasing errors.

5. ANALYTIC SOLUTIONS TO A FOUR-COMPONENT SYSTEM

Although the essential elements of non-linear instability are apparently removed by use of a quadratic-conserving spatial differencing scheme, there remains the question of stability related to time differencing. The usual centered explicit mid-point rule is easily shown to be stable to linear perturbations, if the time step is sufficiently small. Experience indicates, nevertheless, that non-linear solutions tend to become decoupled at adjacent time steps and eventually lose all coherence and/or become catastrophically unstable. Since the truncated wave space systems of (4.3) or (4.6) are exactly equivalent to spatial difference equations applied to a particular form of initial condition, an investigation of stability properties of these systems should be pertinent to the more general problem. In the following development we obtain analytic solutions to the four-component system of (4.6). Similar solutions can be found to (4.5) and to the two-component systems.

The kinetic energy and squared vorticity conservation relations may be obtained from (4.6) in the form

$$A^2 + \frac{3}{2} B^2 + \frac{5}{4} C^2 + \frac{7}{2} D^2 = E^2 = \text{constant} \quad (5.1)$$

$$A^2 + \frac{9}{4} B^2 + \frac{25}{8} C^2 + \frac{49}{4} D^2 = Z^2 = \text{constant}.\quad (5.2)$$

Upon introduction of Δ^2/E and E as scale quantities we obtain from (4.6) the dimensionless equations:

$$\frac{da}{d\vartheta} = -bc - \frac{1}{3} cd \quad (5.3a)$$

$$\frac{db}{d\vartheta} = ac \quad (5.3b)$$

$$\frac{dc}{d\vartheta} = -\frac{2}{5}ab + \frac{2}{3}ad \quad (5.3c)$$

$$\frac{dd}{d\vartheta} = -\frac{1}{7}ac \quad (5.3d)$$

where $Ea=A$, $Eb=B$, $Ec=C$, $Ed=D$, $\frac{4}{\sqrt{3}}\frac{\Delta^2}{E}\vartheta=t$. The

scaled conservation relations now become:

$$a^2 + \frac{3}{2}b^2 + \frac{5}{4}c^2 + \frac{7}{2}d^2 = 1 \quad (5.4a)$$

$$a^2 + \frac{9}{4}b^2 + \frac{25}{8}c^2 + \frac{49}{4}d^2 = z^2 = \frac{Z^2}{E^2}. \quad (5.4b)$$

To solve equations (5.3) we first note that (5.3b and d) imply a linear relationship between b and d , i.e.,

$$d = (b_0 - b)/7 \quad (5.5)$$

where b_0 is a constant. Upon substitution of (5.5) into (5.4) and after some further algebra we obtain the relations

$$a^2 = \frac{20}{21} \left[P^2 - \left(b + \frac{b_0}{20} \right)^2 \right] \quad (5.6a)$$

$$c^2 = \frac{52}{105} \left[Q^2 - \left(b - \frac{5b_0}{26} \right)^2 \right] \quad (5.6b)$$

where

$$P^2 = \frac{7}{4} - \frac{7}{10}z^2 + \frac{11}{200}b_0^2$$

$$Q^2 = -\frac{14}{13} + \frac{14}{13}z^2 - \frac{15}{26} \cdot \frac{7}{26}b_0^2$$

We now introduce (5.6) into (5.3b) to obtain a single integrable equation:

$$\frac{db}{d\vartheta} = \pm \frac{4\sqrt{13}}{21} \sqrt{\left[\left(b + \frac{b_0}{20} \right)^2 - P^2 \right] \left[\left(b - \frac{5b_0}{26} \right)^2 - Q^2 \right]}. \quad (5.8)$$

Certain substitutions described in Whittaker and Watson [25] (chap. XXII), allow reduction of (5.8) into a standard elliptic integral form with the solution for most cases given in the standard Jacobian elliptic function notation by:

$$\frac{b - \xi - \frac{37b_0}{520}}{b - \eta - \frac{37b_0}{520}} = -\sqrt{\frac{P+Q+2\xi}{P+Q+2\eta}} dn(\varphi, k) \quad (5.9)$$

where

$$\varphi = \frac{2\sqrt{13}}{21} \sqrt{(P+Q-2\eta)(P+Q+2\xi)}$$

$$k^2 = 1 - \left(\frac{P+Q-2\xi}{P+Q-2\eta} \right) \left(\frac{P+Q+2\eta}{P+Q+2\xi} \right)$$

$$\left. \begin{matrix} \xi \\ \eta \end{matrix} \right\} = \frac{63b_0}{520} \frac{P-Q}{P+Q} \pm \sqrt{PQ \left[1 - \left(\frac{63}{260} \frac{b_0}{P+Q} \right)^2 \right]}$$

It can be shown that the magnitudes of ξ and η are less than $(P+Q)/2$ and therefore that k is real. If the quantity inside the square root in the expressions for ξ and η is negative, solutions may be written similarly but with Q replaced everywhere by $-Q$. Special solutions arise in the following cases:*

$$P+Q = \frac{63}{260} |b_0| \quad P=0 \quad Q=0 \quad P=Q \quad \text{and} \quad b_0=0 \quad (5.10)$$

The first of these special solutions is always sinusoidal, the second and third constant, and the last is always exponentially damping. The solution for the last case, one of particular interest here, is obtained by direct integration of (5.8) and is.

$$b = \pm P \tanh \left(\frac{4\sqrt{13}}{21} P\vartheta \right) = -7d$$

$$|a| = \sqrt{\frac{20}{21}} \operatorname{sech} \left(\frac{4\sqrt{13}}{21} P\vartheta \right) = \frac{25}{13} |c| \quad (5.11)$$

where

$$P = \sqrt{7/11}$$

thus

$$|b| \rightarrow \sqrt{7/11}, \quad |d| \rightarrow \sqrt{7/11}/7, \quad |a|, |c| \rightarrow 0 \text{ as } \vartheta \rightarrow \infty.$$

It is easily shown that the asymptotic solutions lie along four lines in the a, b, c phase volume (d is not independent, because of (5.4 a)). They thus constitute a set of measure zero and have no probability of arising from initially random choices of a, b , and c .

As indicated previously, solutions to (4.5), arising from analytic spatial derivatives, are similar in form to the above but with different numerical coefficients. Again all are periodic with the exception of a single asymptotic case. Somewhat simpler but closely related periodic and asymptotic solutions also exist for two-component systems like (4.3). The following investigations of the behavior of solutions of the finite time difference equations analogous to the four component system obtained from J_A thus will also be pertinent to the two-component systems like (4.3) obtained by use of J_2 and J_3 .

6. FINITE TIME-DIFFERENCE SOLUTIONS

As shown in section 3, Fourier analysis of the original partial differential equation (2.1), with the spatial derivatives replaced by one of the quadratic-conserving finite difference expressions, converts it into a closed set of quadratic-conserving ordinary first-order differential

*Another special case, $P=Q < \frac{63}{520} |b_0|$ is not allowed because of limitations on the magnitude of real variables imposed by (5.4 a).

equations. Methods of numerical solution of such equations are rather well developed, in contrast to the case with the original partial differential equations. The fourth order Runge-Kutta method, for example, combines high accuracy, stability, and relatively straightforward machine programming. It is not entirely clear why such methods have been generally neglected in the time differencing of the partial differential systems, but perhaps the best reason is that time differencing errors have previously been considered negligible compared to the serious stability problems associated with non-linear spatially differenced terms. With the introduction of the quadratic-conserving schemes described above, time differencing errors take on a new importance. Several calculations performed using these schemes, including those by Deardorff, Bryan, and Mintz and Arakawa (all from personal communication), exhibited a slow instability apparently associated with the time integration method. An approach to understanding this instability is obtainable from consideration of a limited component system. Much of the following analysis utilizes the terminology and notation of Henrici [10].

Consider the following system of ordinary differential equations for the dependent variables x_i , functions of t :

$$\frac{dx_i}{dt} = f_i(x_1, x_2, \dots, t) \quad (6.1)$$

where solutions are sought satisfying the initial conditions

$$x_i(0) = \eta_i \quad (6.2)$$

Among the discrete variable methods for the solution of such a set we can distinguish between one-step and multi-step methods. In a one-step method the values of x_i at each time increment can be found if only the values at the previous increment are known. In a multi-step method the calculation of a new time increment of x_i requires knowledge of more than one of the previous values. Another method of classification of methods is by their order of accuracy. In a method of j th order accuracy the Taylor series for the finite difference equation is identical with (6.1) up to and including the term multiplied by the j th power of the time increment. A third classification distinguishes explicit from implicit methods. In the latter the functions f_i must be evaluated at the new time step, generally by some iterative method. Questions of computational stability for a given method depend considerably on its position with respect to each of these classifications.

Most meteorological and oceanographic calculations have been performed with explicit methods of first or second order accuracy. Implicit methods can be justified in order to allow larger time steps in cases wherein a high signal velocity is present in the differential equations but is of no physical interest. There seems to be little point, however, in pursuing a higher order of time accuracy than is present in the spatial derivatives for advectively con-

ditioned flow patterns. Both single-step and multi-step methods are in common use. In this section we investigate the stability and accuracy of several of these methods, listed in table 1, along with one method, that of Adams and Bashforth, having certain advantages apparently overlooked by most previous investigators. The theoretical results have been verified or illustrated by extended integrations of equations (5.3a-d) for some of the methods listed.

Perhaps the most commonly used method in numerical forecasting and related computations is the mid-point rule, also known as the "step-over" (Richardson [20], p. 150) or "leapfrog" (Richtmyer [21]) method. For the initial step Euler's method is commonly used although more sophisticated methods have often been applied. We now derive some results relating to the stability of this method as applied to equations (6.1) for a single variable x , with a linear complex function f specified as

$$f = (u + iv)x \quad (6.3)$$

where u and v are real constants. The analytic solution of (6.1), (6.2), and (6.3) is exponential if $v=0$ and sinusoidal if $u=0$. For the latter case, we can write the solution of difference equation (2) in table 1 as follows:

$$x^{(n)} = \eta_1 e^{in\vartheta} + (-1)^n \eta_2 e^{-in\vartheta} \quad (6.4)$$

where $\tan \vartheta = v\Delta t / [1 - (v\Delta t)^2]^{1/2}$ and the superscript (n) refers to the time level. The amplitude coefficients η_1 and η_2 are obtained by use of Euler's method for the initial time step, and are

$$\eta_1 = \frac{1}{2}[1 + \sqrt{1 - (v\Delta t)^2}] \eta, \quad \eta_2 = \frac{1}{2}[1 - \sqrt{1 - (v\Delta t)^2}] \eta \quad (6.5)$$

The analytic solution is given by

$$x = \eta e^{iut} \quad (6.6)$$

From comparison of (6.4) and (6.6) it is clear that the second term of the former is the spurious solution introduced by the difference approximation. It consists of a single-time-step oscillation modulated by the period of the real solution, and starts and remains with small amplitude, provided $|v\Delta t| \ll 1$. On the other hand, if $v=0$ and $u < 0$ the finite difference solution is

$$x^{(n)} = \eta_1 e^{-n\vartheta} + (-1)^n \eta_2 e^{n\vartheta}, \quad \tanh \vartheta = |u|\Delta t / \sqrt{1 + (u\Delta t)^2}$$

$$\eta_1 = [1 + \sqrt{1 + (u\Delta t)^2}] / 2, \quad \eta_2 = [1 - \sqrt{1 + (u\Delta t)^2}] / 2 \quad (6.6)$$

which is to be compared with the analytic solution

$$x = \eta e^{ut} \quad (6.7)$$

Here we see that the spurious oscillatory part of the solution, again associated with η_2 , grows with time exponentially. This form of computational instability is often associated with diffusion terms. Henrici terms it *weak* instability and shows that it is essentially confined to

TABLE 1.—*Characteristics of methods of integrating first order spectral differential equations*

| Method | Steps | Order | Formula | Explicit or Implicit | Amplification for periodic solution |
|--------------------------|-------|-------|---|----------------------|---|
| 1. Euler..... | 1 | 1 | $x^{(n+1)} = x^{(n)} + f^{(n)} \Delta t$ | E | $(1+p^2)^{1/2}$ |
| 2. Mid-point rule..... | 2 | 2 | $x^{(n+1)} = x^{(n-1)} + 2f^{(n)} \Delta t$ | E | 1 |
| 3. Euler's modified..... | 1 | 2 | $x^{(n+1)} = x^{(n)} + \frac{1}{2}[f^{(n)} + f^{(n+1)}] \Delta t$ | I | 1 |
| 4. Heun..... | 1 | 2 | $\begin{cases} x^{(n+1)*} = x^{(n)} + f^{(n)} \Delta t \\ x^{(n+1)} = x^{(n)} + \frac{1}{2}[f^{(n)} + f^{(n+1)*}] \Delta t \end{cases}$ | E | $(1+p^2/4)^{1/2}$ |
| 5. Matsuno..... | 1 | 1 | $\begin{cases} x^{(n+1)*} = x^{(n)} + f^{(n)} \Delta t \\ x^{(n+1)} = x^{(n)} + f^{(n+1)*} \Delta t \end{cases}$ | E | $(1-p^2+p^4)^{1/2}$ |
| 6. Miyakoda..... | 3 | 2 | $\begin{cases} (\beta + \frac{1}{2})x^{(n+1)} = 3\beta x^{(n)} + (\frac{1}{2} - 3\beta)x^{(n-1)} + \beta x^{(n-2)} + f^{(n)} \Delta t \\ \beta > 0 \end{cases}$ | E | $(1+\beta p^4 + \dots)^{1/2}$ |
| 7. Adams-Bashforth..... | 2 | 2 | $x^{(n+1)} = x^{(n)} + [\frac{3}{2}f^{(n)} - \frac{1}{2}f^{(n-1)}] \Delta t$ | E | $(1+p^4/4 + \dots)^{1/2}$ |
| 8. Lax-Wendroff..... | 2 | 2 | $\begin{cases} x_i^{(n+1)} = x_i^{(n)} + f_i^{(n)} \Delta t - \frac{1}{2}k_x^2 x_i^{(n)} \\ x_i^{(n+2)} = x_i^{(n)} + 2f_i^{(n+1)} \Delta t \end{cases}$ | E | $[1-4p^2(2k_1^2 - k_2^2) + 4p^4]^{1/4}$ |

a class of multi-step difference methods which allow more than one solution to the equation $dx/dt=0$. Neither the single-step methods nor the Adams-Bashforth or Adams-Moulton (implicit) multi-step methods exhibit this form of instability.

These results can be applied to non-linear equations like (5.3) when we recognize that the elliptic integral functions, although generally periodic, partake of the nature of both sinusoidal and exponential forms, as can be seen by examining the first and last of the limiting forms of (5.10). For the latter of these, one may linearize the finite difference equations and find perturbation solutions which are unstable for integrations made by the mid-point rule. It may be expected, therefore, that initial conditions chosen to be close to those of the limiting asymptotic case will lead to instability of the weak time-splitting type. To test this assumption, numerical solutions of (5.3) were obtained using the Euler method for the first step and the mid-point rule for 999 subsequent time increments, or until instability ensued. The following three sets of initial conditions were used:

- (1) $a=0.7664163$, $b=0.14$, $c=0.5526707$, $d=-0.02$
- (2) $a=0.7669696$, $b=0.14$, $c=0.5530697$, $d=0.0$
- (3) $a=0.5$, $b=1/\sqrt{6}$, $c=1/\sqrt{5}$, $d=1/\sqrt{14}$

The first of these corresponds to the asymptotic solution and the second to a small perturbation from it. The third was chosen to have energy uniformly dispersed among all components.

Figures 1, 2, and 3 are time plots of these solutions for the variables a , b , c , and d at odd and even time steps. The time interval is 0.2 non-dimensional unit. All the solutions correspond very accurately to their analytic counterparts as long as the time splitting is small. The curves for case (1) and (2) are almost indistinguishable up to the point where the former becomes unstable, but the latter then becomes periodic with a period agreeing to within about 1 percent of the analytic prediction.

Noticeable splitting occurs periodically as the integration proceeds, and after about 800 time steps the system has reached a point of incipient instability. Figures 4 and 5 show the kinetic energy for odd and even time steps of cases (1) and (2), integrated by the mid-point rule, and case (1) integrated by other schemes to be described. Time-step splitting obviously occurs and amplifies considerably before the average noticeably deviates from unity. In case (3) the oscillations have become shorter and simpler, although far from sinusoidal, and are predictable to an accuracy of 0.5 percent. The splitting here has an amplitude of about 1 percent, too small to plot, and is completely innocuous to at least 1000 time steps. The kinetic energy (not plotted) is essentially constant. This behavior would presumably characterize solutions for the majority of initial conditions chosen at random from all possible values.

Table 1 presents some pertinent details on the remaining methods investigated. Most of the methods, when applied to integration of the equation $dx/dt=ivx$, yield complex exponential solutions. Column 6 shows the amplification factor associated with the real part of this complex exponent, where $p=v\Delta t$.

Euler's method and the mid-point rule have already been discussed. It has long been known that Euler's method leads to slow amplification of oscillating solutions as well as significant phase errors. Euler's modified method, the best known implicit method, is rather ideal in several respects, as it is the only one of those discussed here in which the conservation relations (5.4a, b) hold exactly. Veronis [24] has recently used it for integration of spectral component equations. The Heun method, used by Lorenz [16] and others, is a single-step method which may be considered a first iterative approximation to Euler's modified method. Table 1 shows that periodic solutions amplify, but only by a fourth-order term. Lorenz has shown a similar result for general systems of

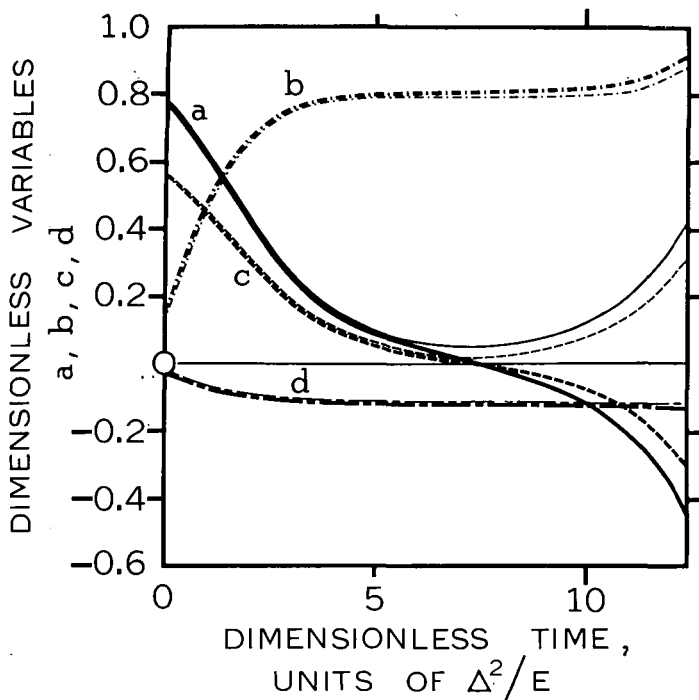


FIGURE 1.—Case 1, asymptotic solution for the dimensionless amplitude coefficients a , b , c , and d , integrated from equation (5.3) by the mid-point rule with time interval 0.2 dimensionless units. The light and heavy curves connect values for odd and even numbered time steps, respectively, after the initial single uncentered step.

conservation equations. Another single-step method proposed by Matsuno (unpublished) and used by Mintz and Arakawa [17] is essentially the first approximation to a first-order backward difference scheme. The amplification factor, like that of Euler's method, differs from unity in a second-order term, but tends to damp all oscillations except the shortest. Equations (5.3) were numerically integrated by this method for the conditions of case (1) which led to instability with the mid-point rule. The kinetic energy, plotted in figure 4, shows clearly the effect of this damping. The step-like appearance of this curve is associated with the slowly oscillatory nature of the numerical solution. This oscillation is itself a truncation error effect, since the analytic solution is asymptotic. It occurs, however, in all the numerical solutions obtained, and is clearly related to the singular nature of the asymptotic case.

Miyakoda [18] (p. 133) suggested use of a three-step method which is essentially redundant, since it is only of second-order accuracy. The redundancy is applied to elimination of weak instability and is most effective when the coefficient β is at or near $1/6$, the value giving optimal damping of the two spurious computational modes. Truncation error increases with β , as does the amplification of the periodic solution shown in column 6 of table 1. For $\beta=0$ the method reduces to the mid-point rule. Numerical integrations were performed for

the optimal value of β and for $\beta=1/4$, the value suggested by Miyakoda, and results for the kinetic energy are plotted, in an expanded scale, on figure 5. There is obviously some oscillation, in phase with an observed oscillation of the basic solution components, but the overall trend is virtually undetectable even after 1000 time steps. Essentially similar results appear for the Adams-Bashforth method, also presented on figure 5. A slight trend toward increasing energy is detectable here, as could be expected from the somewhat larger amplification factor compared to Miyakoda's method. This method is somewhat simpler than Miyakoda's and more efficient than Heun's. It has not, to my knowledge, been previously used in numerical forecasting.

The scheme proposed by Lax and Wendroff [13] is of a slightly different nature than those considered above, as it was originally designed for application to partial differential equations.

The principal identifying feature of the scheme seems to be in the time differencing, however. Elsewhere in this issue Kasahara [11] and Fischer [7] discuss the stability of difference schemes closely related to that of Lax and Wendroff but differing somewhat in the space-time lattice structure. Here we consider the Lax-Wendroff scheme applied to equation (2.1), but modified by use of the Arakawa spatial Jacobian J_A . As shown by Richtmyer [21] the scheme may be written as a two-step process as follows

$$\begin{aligned}\zeta^{(n+1)} &= \zeta^{(n)} + \frac{\Delta^2}{4} \nabla^2 \zeta^{(n)} - J_A^{(n)} \cdot \Delta t \\ \zeta^{(n+2)} &= \zeta^{(n)} - 2J_A^{(n+1)} \cdot \Delta t.\end{aligned}\quad (6.8)$$

The five-point Laplacian operator appearing in the first step arises because of the spatial averaging employed by Lax and Wendroff, and seems to be an essential feature of the system, although in Kasahara's schemes it appears to have a coefficient only one-half as large. Upon application of the Fourier transform to (6.8) the system defined in column 4 of table 1 is obtained, where the k_i 's are sines of wave numbers. Except for the pseudo-viscous damping caused by the Laplacian term this scheme is similar in nature and accuracy to the Heun method and is known in the literature as the "improved polygon" method (Henrici [10], Collatz [4]). The presence of the damping terms, however, causes extremely large errors in the treatment of high wave number components.

The results of the numerical integration of (5.3) by this modified Lax-Wendroff method are, therefore, essentially nonsense, as can be seen by viewing the energy curve in figure 4. While this may not be an entirely fair manner of evaluation, it does show that high wave numbers are handled with effectively no accuracy by this method. One may of course argue, from the previous analysis of truncation errors of equation (4.6), that there is very little accuracy in the high wave number results for any

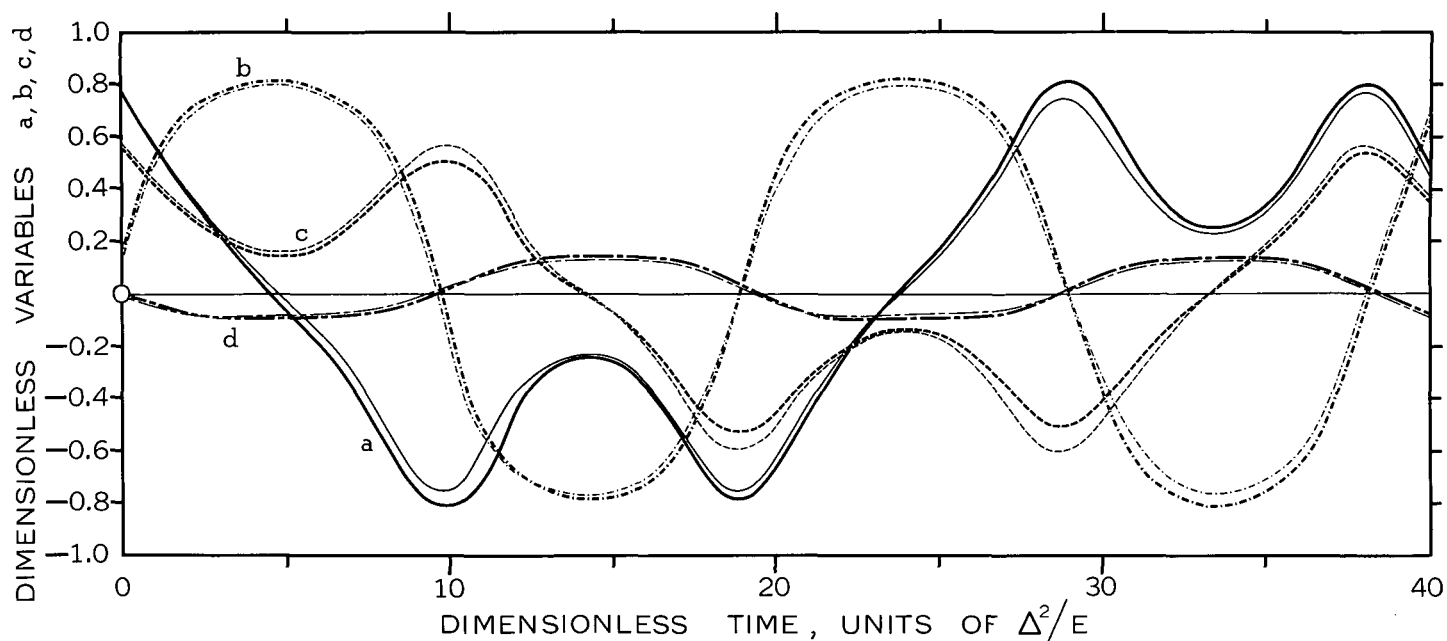


FIGURE 2.—Case 2, perturbation from asymptotic solution. See figure 1 caption for other details.

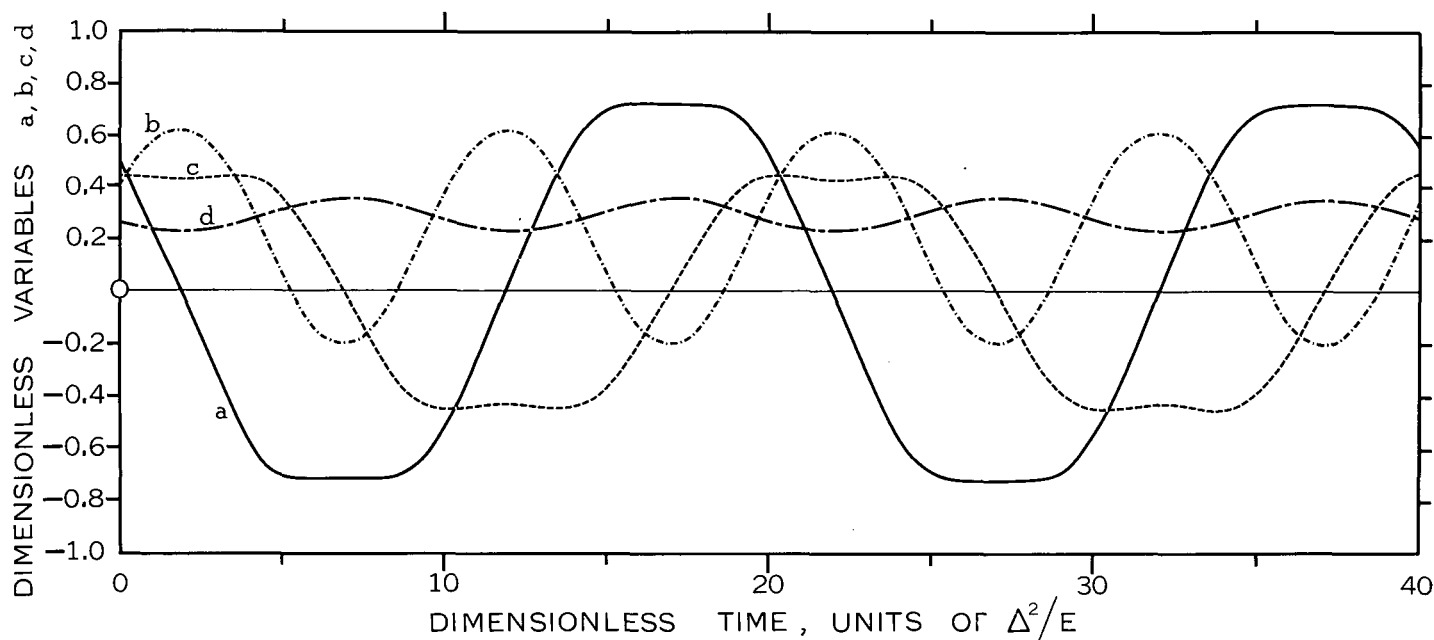


FIGURE 3.—Case 3, uniform energy dispersion. See figure 1 caption for other details.

second-order method. It should also be noted that the modified Lax-Wendroff schemes discussed elsewhere in this issue by Kasahara [11] and Fischer [7] are substantially better in this respect because of the time-space grid staggering of variables. The finite Laplacian operator in (6.8) would then be replaced by a similar expression taken over one-half of a grid interval and the damping effects would be considerably less.

7. CONCLUSIONS AND OUTLOOK

By expressing the stream function in a finite Fourier series we have derived the spectral interaction matrices corresponding to the finite difference Jacobian forms previously obtained by Arakawa [1] and Fromm [8]. Comparison of the interaction coefficients with those of the analytic Jacobian showed that the truncation errors

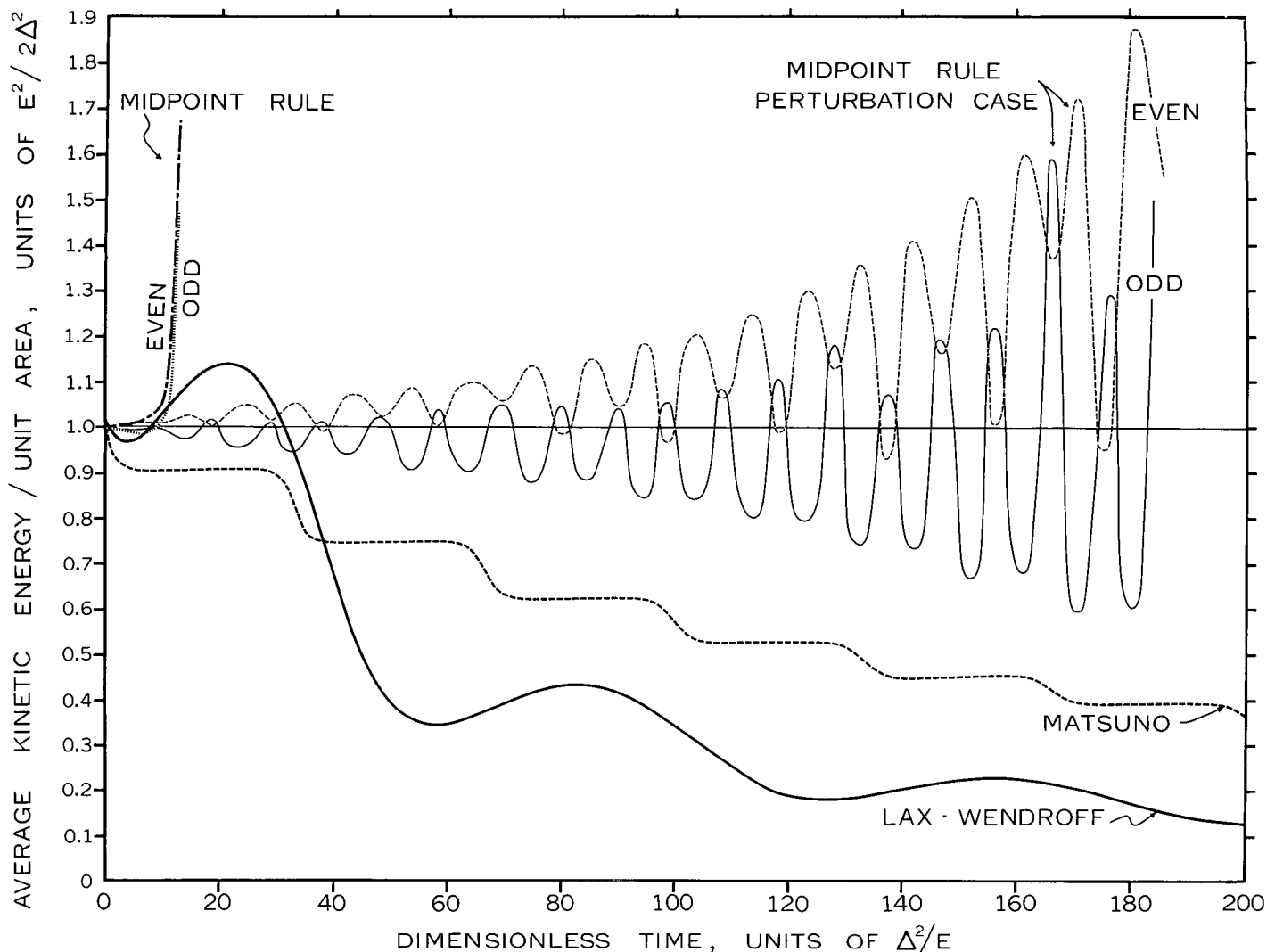


FIGURE 4.—Dimensionless normalized energy as a function of time for various initial conditions and numerical solution methods. The separation between odd and even numbered time steps shows the development of instability in the mid-point rule calculations.

are of three types, only two of which are reducible by higher order differencing. The third type, the aliasing error, is present in all of the Jacobian forms considered but does not lead to computational instability in any of the quadratic-conserving forms because of the balancing of spurious interactions in triads. Specific examples of truncated spectral systems were considered to illustrate this effect and to compare the behavior of the various quadratic-conserving formulations.

The remaining factor leading to possible computational instability in a simple non-linear vorticity equation, the time differencing, was investigated by comparison of analytic and numerical solutions of a four-component finite-difference spectral equation system. From theoretical consideration and integration of a limited number of cases it appeared that the mid-point rule usually applied in meteorological calculations is unstable for certain rather special sets of initial conditions. Instability, when it occurs, is of the nature of an amplifying single-time-

step oscillation. Several alternate methods of stabilizing the calculations were tested analytically or experimentally. All exhibited improved stability, and three, the Heun, Miyakoda, and the simple and rather efficient Adams-Bashforth method seemed to have acceptable, and roughly equal, accuracy.

In most practical or theoretical initial value problems to which numerical methods are applied, the equations, variables, coordinates, and/or boundary conditions exhibit greater complexities than are in (2.1). Each problem must be considered on its own terms, and it is not implied that use of a quadratic-conserving Jacobian plus stable second-order accuracy time differencing will solve all stability problems. These systems can, however, be generalized to cover a considerable range of variation of the systems of equations, boundary conditions, and mapping factors. As an example, a 9-level general circulation model now being used by Smagorinsky and Manabe of the Weather Bureau's General Fluid Dynamics

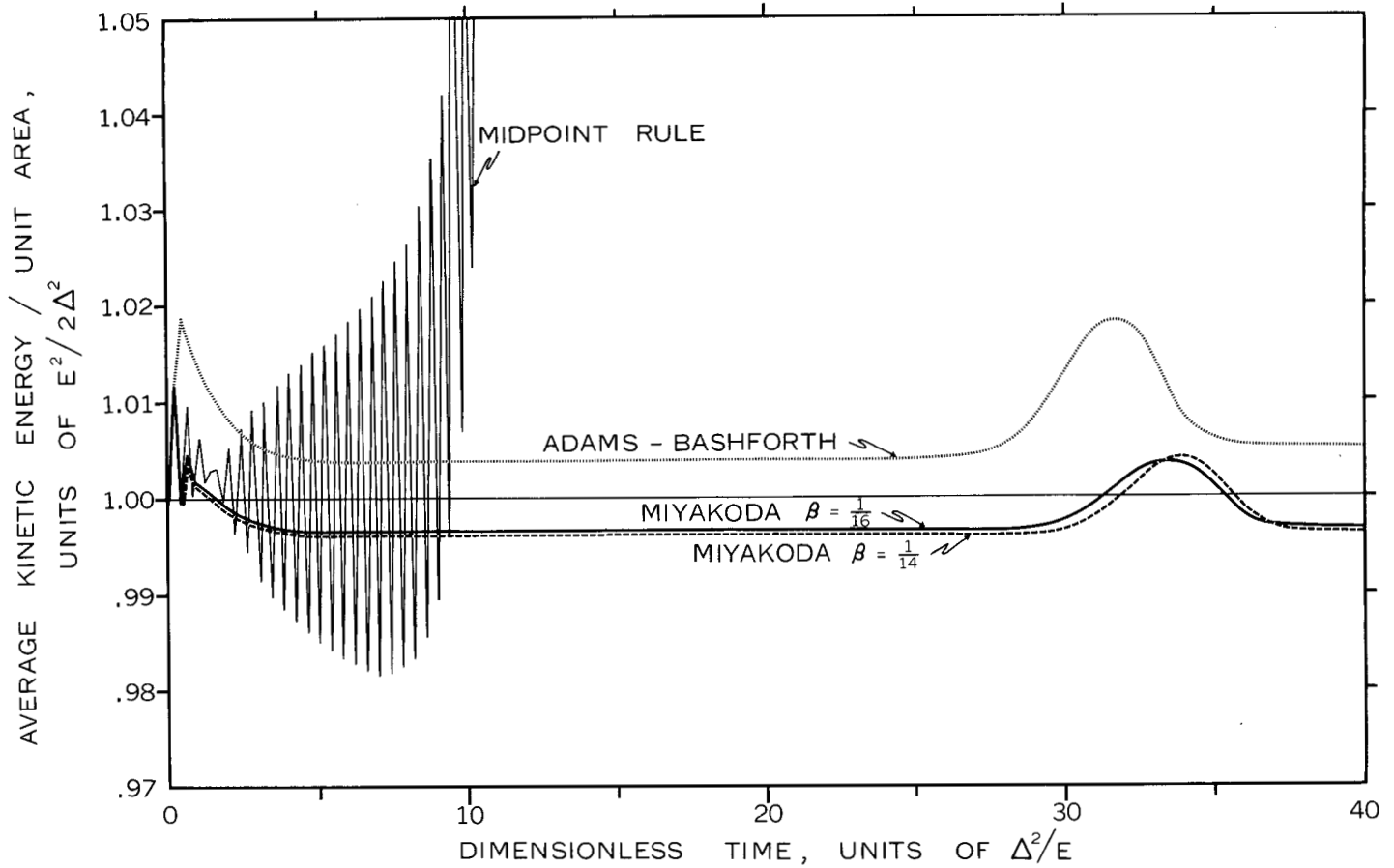


FIGURE 5.—Dimensionless normalized energy, plotted on a more open scale. Values for odd and even time steps are joined to show the contrast between the mid-point rule and the more stable methods.

Laboratory has been recently reformulated to incorporate these methods.

APPENDIX

A Systematic Derivation of the Quadratic-Conserving Finite Representations of the Jacobian

Let ψ and ζ be dependent variables represented at the points $x=m\Delta$, $y=n\Delta$. We introduce the shorthand notation

$$\psi_{mn} = \psi(x, y), \quad \zeta_{mn} = \zeta(x, y). \quad (\text{A1})$$

We now denote by J_{mn} a finite sum of product terms, whose factors are chosen from a 9-point box surrounding the point x, y .

$$J_{mn} = \sum_{l=-1}^1 \sum_{k=-1}^1 \sum_{j=-1}^1 \sum_{i=-1}^1 a_{ijkl} \psi_{m+i, n+j} \zeta_{m+k, n+l} \quad (\text{A2})$$

where a_{ijkl} is one of 81 components of a fourth order tensor. We require that a_{ijkl} be specified to satisfy certain properties of the analytic Jacobian, $J(\psi, \zeta)$.

If the x and y axes are rotated by a multiple of $\pi/2$ the analytic Jacobian is unchanged, while its sign is reversed

if x is replaced by $-x$ or y by $-y$. These requirements of rotational symmetry and reflective anti-symmetry lead to the coefficient relations

$$a_{ijkl} = a_{j-il-k} = a_{-i-j-k-l} = a_{-ji-lk} \quad (\text{A3})$$

$$a_{ijkl} = -a_{-ij-k-l} = -a_{i-j-k-l} = a_{-i-j-k-l}. \quad (\text{A4})$$

The above relations lead to vanishing of 33 of the coefficients, e.g., $a_{1111} = a_{1-11-1} = -a_{-1-11-1} = 0$. Of the remaining 48 only 6 are independent. For simplicity we renumber these a_1 to a_6 as follows:

$$\begin{aligned} a_1 &= a_{1001} = a_{01-10} = a_{-100-1} = a_{0-110} \\ &= -a_{100-1} = -a_{0110} = -a_{-1001} = -a_{0-1-10} \\ a_2 &= a_{1011} = a_{01-11} = a_{-10-11} = a_{0-11-1} \\ &= -a_{101-1} = -a_{0111} = -a_{-10-11} = -a_{0-1-1-1} \\ a_3 &= a_{1101} = a_{-11-10} = a_{-1-10-1} = a_{1-110} \\ &= -a_{1110} = -a_{-1101} = -a_{-1-1-10} = -a_{1-10-1} \\ a_4 &= a_{10-11} = a_{01-1-1} = a_{-101-1} = a_{0-111} \\ &= -a_{10-1-1} = -a_{011-1} = -a_{-101-1} = -a_{0-1-11} \\ a_5 &= a_{11-11} = a_{-11-1-1} = a_{-1-11-1} = a_{1-111} \\ &= -a_{111-1} = -a_{-1111} = -a_{-1-1-11} = -a_{1-1-1-1} \\ a_6 &= a_{11-10} = a_{-110-1} = a_{-1-110} = a_{1-101} \\ &= -a_{110-1} = -a_{-1110} = -a_{-1-101} = -a_{1-1-10}. \end{aligned} \quad (\text{A5})$$

In order that J_{mn} be a second order approximation to J we expand ψ and ζ in a Taylor's series around $x=m\Delta$, $y=n\Delta$, i.e.:

$$\psi_{m+i, n+j} = \psi_{mn} + \Delta \left(i \frac{\partial \psi_{mn}}{\partial x} + j \frac{\partial \psi_{mn}}{\partial y} \right) + \frac{\Delta^2}{2!} \left(i^2 \frac{\partial^2 \psi_{mn}}{\partial x^2} + 2ij \frac{\partial^2 \psi_{mn}}{\partial x \partial y} + j^2 \frac{\partial^2 \psi_{mn}}{\partial y^2} \right) + \dots \quad (\text{A6})$$

$$\zeta_{m+k, n+l} = \zeta_{mn} + \Delta \left(k \frac{\partial \zeta_{mn}}{\partial x} + l \frac{\partial \zeta_{mn}}{\partial y} \right) + \frac{\Delta^2}{2!} \left(k^2 \frac{\partial^2 \zeta_{mn}}{\partial x^2} + 2kl \frac{\partial^2 \zeta_{mn}}{\partial x \partial y} + l^2 \frac{\partial^2 \zeta_{mn}}{\partial y^2} \right) + \dots \quad (\text{A7})$$

Upon substitution of (A6) and (A7) into (2.1) and equating coefficients of the derivatives, a new relation is obtained, which may be defined as the second order accuracy criterion:

$$a_1 + a_2 + a_3 + a_4 + 2a_5 + a_6 = 0 \quad (\text{A8})$$

We now apply the linear and quadratic conservation requirements. These may be stated as the reduction of area integrals to line integrals around a boundary. For conservation of vorticity, kinetic energy, and squared vorticity, this means that the summations

$$\sum_{n=-1}^1 \sum_{m=-1}^1 J_{mn}, \quad \sum_{n=-1}^1 \sum_{m=-1}^1 \psi_{mn} J_{mn}, \quad \sum_{n=-1}^1 \sum_{m=-1}^1 \zeta_{mn} J_{mn}$$

must include, respectively, no contributions from the m, n point.

Figure 6 is a schematic diagram intended to illustrate some of the interaction coefficient properties. The axes are in the x and y directions with the origin at the point $x=m\Delta$, $y=n\Delta$. The solid arrows represent interaction coefficients connecting vorticity, ζ , at the arrowhead and stream function, ψ , at the tail, e.g., $a_1 = a_{1001}$, $a_3 = a_{1101}$, etc. The dashed line arrows represent the same coefficients acting on variables displaced one or two grid intervals in the vertical and/or horizontal, but they are labeled according to their value in the grid centered at m, n . The vorticity conservation condition requires that the sum of the coefficients associated with parallel equal length arrows running in the same direction must vanish. For most of those appearing in figure 6 this is already the case, e.g., $a_1 - a_1 = 0$, $a_2 - a_2 + a_3 - a_3 = 0$, in which it may be noted that all interactions involving the origin were made to vanish by the symmetry conditions in (A3) and (A4). The only new relation arising from this condition arises from equating the two sets of long diagonal interaction arrows, i.e.

$$a_4 = a_6 \quad (\text{A9})$$

In order to derive the quadratic conservation properties, we represent triad interactions by a triangle, with one vertex at the center and the opposite side given by the interaction coefficient arrow. Thus the kinetic energy

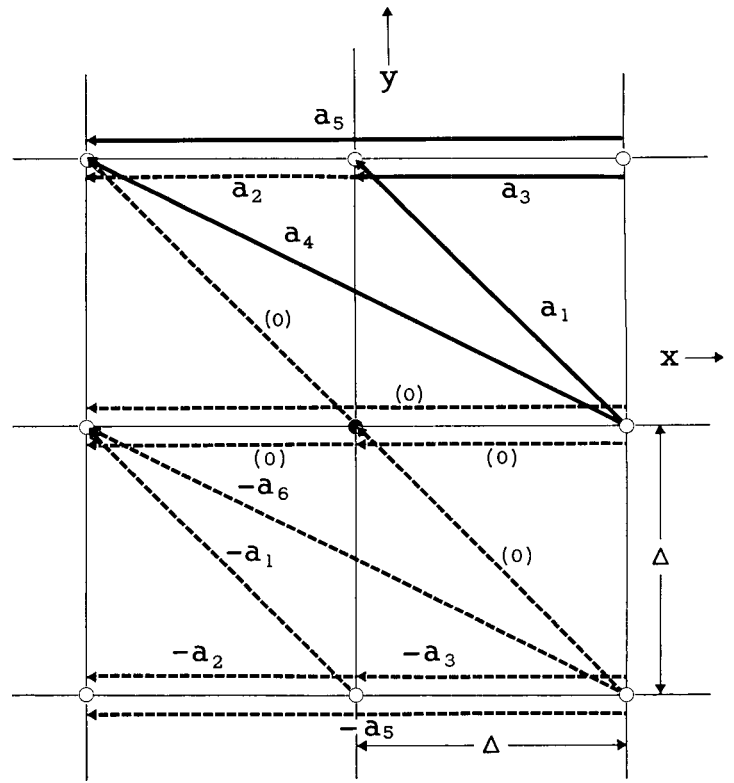


FIGURE 6.—Interaction coefficient diagram. The open circles are grid points from which stream function and vorticity contribute to the Jacobian evaluated at the origin (solid circle). The arrows represent interaction coefficients connecting stream function at the tail and vorticity at the head, labeled according to (A5). The solid arrows all start in the upper right quadrant while the dashed ones are all parallel and congruent to them.

triad $a_{01-11}\psi_{mn+1}\zeta_{m-1, n+1}\psi_{mn}$, obtained from multiplication of J_{mn} by ψ_{mn} , is represented by the upper triangle in figure 7, while the triad $a_{0-1-10}\psi_{mn-1}\zeta_{m-1, n}\psi_{mn}$ similarly forms the lower triangle. No other triangles may be formed within the 2Δ square which are congruent, parallel, and whose corners represent the same variables (ψ or ζ). Thus the sum of these paired interaction coefficients must vanish, i.e., $a_{01-11} - a_{0-1-10} = 0$, in order that kinetic energy be conserved within the square. Other triangles may be formed using the other interaction arrows represented by figure 6. Most of these have no pairings, and the interaction coefficients must therefore vanish. The result, for the energy conservation requirement, is that:

$$a_1 = a_2, \quad a_4 = a_5 = a_6 = 0 \quad (\text{A10})$$

while similar pairings for the product of J_{mn} and ζ_{mn} yield the relations

$$a_1 = a_3, \quad a_4 = a_5 = a_6 = 0. \quad (\text{A11})$$

Upon application of the second-order accuracy requirement, (A8), one degree of freedom is removed from each of the above and we obtain the formulas

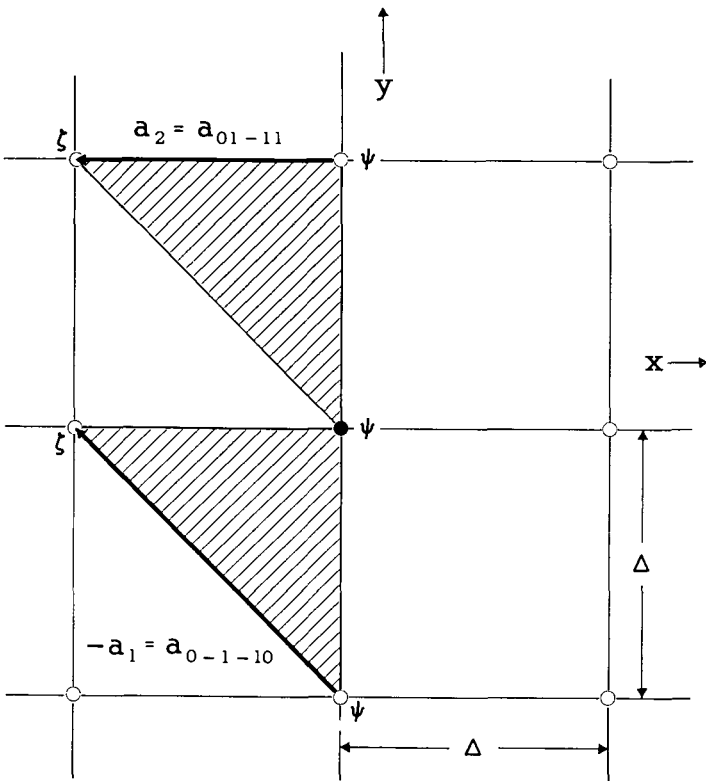


FIGURE 7.—Energy conservation interaction diagram. The hatched triangles represent the interaction products of two stream functions and one vorticity value at their vertices.

$$a_1 = a_2 = \frac{1}{8} - \frac{a_3}{2}, \quad a_4 = a_5 = a_6 = 0 \quad (\text{A12})$$

for kinetic energy conservation, and

$$a_1 = a_3 = \frac{1}{8} - \frac{a_2}{2}, \quad a_4 = a_5 = a_6 = 0 \quad (\text{A13})$$

for squared vorticity conservation. Each of these has one arbitrary coefficient; thus it is possible to satisfy both with the unique system

$$a_1 = a_2 = a_3 = 1/12, \quad a_4 = a_5 = a_6 = 0. \quad (\text{A14})$$

The difference schemes described in the text are obtained from special choices of the arbitrary coefficients. J_1 is the vorticity conserving scheme corresponding to $a_1 = 1/4$, while J_2 is obtained from $a_2 = 1/4$, and J_3 from $a_3 = 1/4$, all other coefficients vanishing. The combined system J_A is obtained from (A14). As stated in the text, any linear combination of J_A with J_1 , J_2 , or J_3 preserves the latter's properties. For example $3J_A/2 - J_3/2 = (J_1 + J_2)/2$, corresponding to $a_1 = a_2 = 1/8$, which satisfies (A12) just as does J_3 .

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